Supplementary Materials

for

A Functional Group Oxidation Model (FGOM) for SOA formation and Aging

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1. Statistical fit of compound vapor pressure

We used 1080 "standard molecules" to obtain the parameters in equation (2). There are 35 sets of different combinations of the four functional groups. For each combination, carbon number ranges from 5 to 14. Alkanes are included with the same carbon number range. In addition, the contribution of straight, branching and cyclic structures to the vapor pressure are also considered. In summary, 1080 "standard compounds" are used for the nonlinear fitting. All are listed in Table S1.

2. Development of the functionlization vs. fragmentation channels in the FGOM

Photooxidation of dodecane under high-NO_x conditions illustrates how the functionlization vs. fragmentation channels are developed in the FGOM model. Figure S2 shows the detailed scheme for the formation of 1st generation products, i.e., C_{12}-(ONO_2), C_{12}-(OH + ONO_2), and C_{12}-(C=O + OH), in addition to the formation of 2nd generation products, i.e., C_{12}-(C=O), C_{12}-(2×ONO_2), C_{12}-(OH + ONO_2), C_{12}-(C=O + OH), C_{12}-(OH + 2×ONO_2), and C_{12}-(C=O + OH + ONO_2), from one of the 1st generation products. The specific chemistry underlying the formation of the C_{12} products in the functionalization channel is discussed in Section 2.1. For the high-NO_x photooxidation of dodecane, the OH reaction rates, the photolysis rate of the –ONO_2 group, together with the branching ratio (obtained from MCM 3.1) for the formation of the RO· radical vs. the –ONO_2 group

from the $RO_2\cdot$ + NO pathway, govern the relative abundances of different functional groups (Figure S2). Note that since the OH concentration generally varies with time over the course of photooxidation, the branching ratios are a function of time. The values shown in Figure S2 correspond to those at the beginning of the photooxidation, when the OH concentration is ~ 1×10^7 molecules cm^{-3}.

Once a certain generation of products is formed, an operator P_f, which is a function of the O:C ratio, is applied to each of the products to calculate the fraction of fragmentation that the product undergoes. Take the 2nd generation product C_{12}-(OH+2×ONO_2) as an example (Figure S3), the best-fit f_v value obtained from the optimization is 0.57, indicating that 26.4% of this product undergoes further functionalization and 73.6% of it fragments, producing a C_1 product, together with a co-product C_{11}-(OH+2×ONO_2). An operator P_f is subsequently applied to this C_{11} product to calculate its fraction of functionalization, via the same reaction mechanism as C_{12}-(OH+2×ONO_2), vs. fragmentation, which generates another C_1 product, together with a co-product C_{10}-(OH+2×ONO_2). Equation (2) in the main text governs the least carbon number for a certain combination of different functional groups that can be produced from the fragmentation channel. Alkoxy ($RO\cdot$) radical fragmentation mechanisms are not incorporated explicitly in the FGOM model. Instead, the operator P_f, which is indicative of the chemical species, is applied to the stable molecules to govern the probablity of fragmentation in an OH-reaction initiated generation.

3. Particle wall loss corrections

The particle wall loss corrected SOA mass data were used as the basis for model fitting. Additional details about particle wall loss correction protocols can be found in Loza et al. (2012). Two limiting assumptions can be made for the interactions between particles on the wall and suspended vapor: 1) particles deposited on the wall are assumed to interact with the suspended vapors as if they had remained suspended and 2) particles deposited on the wall are assumed to cease interaction with the suspended vapors. The first assumption gives the upper bound limit on SOA mass concentration. To invoke this assumption, one applies the time-dependent organic to sulfate ratio measured by AMS to the seed volume concentration measured by DMA. We do not usually use this assumption considering the fact that the presence of organics enhances the collection efficiency of sulfates in AMS. The second assumption is applied in the present study. In this case, particles deposited on the wall remain the same size and do not undergo continued organic growth. In order to calculate the total particle mass lost on the wall as a function of time, the size-dependent particle wall loss rate parameter (β) needs to be determined. Wall loss calibration experiments were carried out by atomizing 1.0 M and 0.015 M ammonium sulfate solution ($(NH_4)_2SO_4$) into the chamber and monitoring the decay of

particle number distribution using a DMA. The size dependent wall loss rate paramter (β) can be obtained by fitting equation S1 to the data for pure wall loss:

$$n_{i,s} = n_{i,0} \times \exp(-\beta t) \quad \text{(Equ S1)}$$

where $n_{i,s}$ is the suspended particle number distribution in size bin i at time t, and $n_{i,0}$ is the initial particle number distribution in size bin i. The β values so derived were then applied to the C_{12} alkane chamber experiments. For each size bin i at each time step j, particle number distribution deposited to the wall ($n_{w,i,j}$) is calculated as:

$$n_{w,i,j} = n_{s,i,j} \times [1 - \exp(-\beta \Delta t)] \quad \text{(Equ S2)}$$

where $n_{s,i,j}$ is the suspended particle number distribution in size bin i at time step j, and Δt is the difference between time step j and time step $j + 1$. The deposited particle size distribution ($n_{w,i,j}$) is added to the suspended particle size distribution ($n_{s,i,j}$) to give the total particle distribution ($n_{tot,i,j}$):

$$n_{tot,i,j} = n_{w,i,j} + n_{s,i,j} \quad \text{(Equ S3)}$$

The total number concentration in size bin i at time step j ($N_{tot,i,j}$) can be calculated by converting the size distribution based on $d(lnD_p)$ to $d(D_p)$:

$$N_{tot,i,j} = n_{tot,i,j} / D_{p,i}\, ln10 \times (D_{p,i+} - D_{p,i-}) \quad \text{(Equ S4)}$$

where $D_{p,i}$ is the median particle diameter for size bin i, $D_{p,i+}$ is the upper limit of particle diameter for size bin i, and $D_{p,i-}$ is the lower limit of particle diameter for size bin i. Assuming spherical particles, the total volume concentration at time step j ($V_{tot,j}$) is:

$$V_{tot,j} = \sum_{i}^{m} \frac{\pi}{6} D_{p,i}^{3} \times N_{tot,i,j} \quad \text{(Equ S5)}$$

The total organic mass growth ($\Delta M_{o,j}$) at time step j is:

$$\Delta M_{o,j} = \rho\,(V_{tot,j} - V_{seed}) \quad \text{(Equ S6)}$$

where ρ, the density for a specific C_{12} alkane SOA under high- or low- NO_x conditions, is obtained from seed free nucleation experiments.

3. HR-ToF-AMS data processing protocols

All AMS data were processed with "Squirrel", the Tof-AMS Unit Resolution Anylysis Toolkit (http://cires.colorado.edu/jimenez-group/ToFAMSResources /ToFSoftware/index. html), in Igor Pro Version 6.22A (Wavemetrics, Lake Oswego, OR). The ToF-AMS High Resolution Analysis software tool PIKA (Peak Integration by Key Analysis) was employed for high-resolution analysis (Decarlo et al., 2006). O:C and H:C ratios were computed using the computation toolbox "Analytical Procedure for Elemental Separation", which applies elemental analysis to the W-mode data. The

interference of chamber air on the particulate spectrum was corrected by adjusting parameters in the fragmentation table based on the "filter run" (AMS is colleting chamber air with a particle filter in-line) before each alkane photooxidation experiment (Chhabra et al., 2010; Craven et al., 2012). Briefly, the ion CO_2^+ signal from ambient CO_2, which is estimated to be 370 ppm in the chamber, is removed to determine the organic contribution of CO_2^+ to m/z 44. The ion CO^+ (m/z 28), which is considered to be a common fragment of organic species, can be overwhelmed by ion N_2^+ signal derived from ambient N_2. In this study, we used the particle-phase ratio of CO^+/CO_2^+ to be unity as the default value to calculate the contribution of CO^+ to the total organic signal. We also checked W-mode, which has higher resolution than V-mode, to separate the CO^+ signal from N_2^+ signal. The $C_2H_4^+$ ion signal was removed because of its interference with the N_2^+ signal. The signals from H_2O^+, OH^+, and O^+ can be biased by water from both gas and particle phase. We use fragmentation table parameters in Aiken et al. (2008) to estimate the organic contributions (H_2O^+ = 22.5%, OH^+ = 5.625, and O^+ = 0.9%). For the high-NO_x alkane data, NO^+ and NO_2^+ signals were included in the O:C calculations because they trend with the organic mass so that they might come from organic nitrates. Including both of these ions increases O:C but does not increase the oxidation state of the carbon backbone (Kroll et al., 2011).

Table S1. Characteristics of the 1080 “standard molecules”

No.	Structure	Carbon Number	Oxygen Number	Nitrogen Number	Functional Groups	Vapor Pressure (atm @ 298 K)
1	Straight	5	0	0	-	6.4849E-01
2	Straight	6	0	0	-	2.1204E-01
3	Straight	7	0	0	-	6.9332E-02
4	Straight	8	0	0	-	2.2670E-02
5	Straight	9	0	0	-	7.4124E-03
6	Straight	10	0	0	-	2.4237E-03
7	Straight	11	0	0	-	7.9248E-04
8	Straight	12	0	0	-	2.5912E-04
9	Straight	13	0	0	-	8.4726E-05
10	Straight	14	0	0	-	2.7703E-05
11	Straight	5	1	0	1-OH	1.3021E-02
12	Straight	6	1	0	1-OH	4.2574E-03
13	Straight	7	1	0	1-OH	1.3921E-03
14	Straight	8	1	0	1-OH	4.5517E-04
15	Straight	9	1	0	1-OH	1.4883E-04
16	Straight	10	1	0	1-OH	4.8664E-05
17	Straight	11	1	0	1-OH	1.5912E-05
18	Straight	12	1	0	1-OH	5.2028E-06
19	Straight	13	1	0	1-OH	1.7012E-06
20	Straight	14	1	0	1-OH	5.5624E-07
21	Straight	5	2	0	2-OH	3.0091E-05
22	Straight	6	2	0	2-OH	9.8391E-06
23	Straight	7	2	0	2-OH	3.2171E-06
24	Straight	8	2	0	2-OH	1.0519E-06
25	Straight	9	2	0	2-OH	3.4395E-07
26	Straight	10	2	0	2-OH	1.1246E-07
27	Straight	11	2	0	2-OH	3.6773E-08
28	Straight	12	2	0	2-OH	1.2024E-08
29	Straight	13	2	0	2-OH	3.9315E-09
30	Straight	14	2	0	2-OH	1.2855E-09
31	Straight	5	3	0	3-OH	5.1505E-08
32	Straight	6	3	0	3-OH	1.6841E-08
33	Straight	7	3	0	3-OH	5.5065E-09
34	Straight	8	3	0	3-OH	1.8005E-09
35	Straight	9	3	0	3-OH	5.8871E-10
36	Straight	10	3	0	3-OH	1.9249E-10
37	Straight	11	3	0	3-OH	6.2941E-11
38	Straight	12	3	0	3-OH	2.0580E-11
39	Straight	13	3	0	3-OH	6.7292E-12
40	Straight	14	3	0	3-OH	2.2003E-12
41	Straight	5	1	0	1-C=O	4.1382E-02

42	Straight	6	1	0	1-C=O	1.3531E-02
43	Straight	7	1	0	1-C=O	4.4243E-03
44	Straight	8	1	0	1-C=O	1.4466E-03
45	Straight	9	1	0	1-C=O	4.7301E-04
46	Straight	10	1	0	1-C=O	1.5466E-04
47	Straight	11	1	0	1-C=O	5.0570E-05
48	Straight	12	1	0	1-C=O	1.6535E-05
49	Straight	13	1	0	1-C=O	5.4066E-06
50	Straight	14	1	0	1-C=O	1.7678E-06
51	Straight	5	2	0	2-C=O	3.7533E-03
52	Straight	6	2	0	2-C=O	1.2272E-03
53	Straight	7	2	0	2-C=O	4.0128E-04
54	Straight	8	2	0	2-C=O	1.3121E-04
55	Straight	9	2	0	2-C=O	4.2901E-05
56	Straight	10	2	0	2-C=O	1.4028E-05
57	Straight	11	2	0	2-C=O	4.5867E-06
58	Straight	12	2	0	2-C=O	1.4997E-06
59	Straight	13	2	0	2-C=O	4.9037E-07
60	Straight	14	2	0	2-C=O	1.6034E-07
61	Straight	5	3	0	3-C=O	4.9317E-04
62	Straight	6	3	0	3-C=O	1.6125E-04
63	Straight	7	3	0	3-C=O	5.2726E-05
64	Straight	8	3	0	3-C=O	1.7240E-05
65	Straight	9	3	0	3-C=O	5.6371E-06
66	Straight	10	3	0	3-C=O	1.8432E-06
67	Straight	11	3	0	3-C=O	6.0268E-07
68	Straight	12	3	0	3-C=O	1.9706E-07
69	Straight	13	3	0	3-C=O	6.4434E-08
70	Straight	14	3	0	3-C=O	2.1068E-08
71	Straight	5	2	0	1-OOH	9.6145E-04
72	Straight	6	2	0	1-OOH	3.1437E-04
73	Straight	7	2	0	1-OOH	1.0279E-04
74	Straight	8	2	0	1-OOH	3.3610E-05
75	Straight	9	2	0	1-OOH	1.0990E-05
76	Straight	10	2	0	1-OOH	3.5933E-06
77	Straight	11	2	0	1-OOH	1.1749E-06
78	Straight	12	2	0	1-OOH	3.8417E-07
79	Straight	13	2	0	1-OOH	1.2561E-07
80	Straight	14	2	0	1-OOH	4.1073E-08
81	Straight	5	4	0	2-OOH	4.9545E-07
82	Straight	6	4	0	2-OOH	1.6200E-07
83	Straight	7	4	0	2-OOH	5.2969E-08
84	Straight	8	4	0	2-OOH	1.7320E-08
85	Straight	9	4	0	2-OOH	5.6631E-09

86	Straight	10	4	0	2-OOH	1.8517E-09
87	Straight	11	4	0	2-OOH	6.0546E-10
88	Straight	12	4	0	2-OOH	1.9797E-10
89	Straight	13	4	0	2-OOH	6.4731E-11
90	Straight	14	4	0	2-OOH	2.1165E-11
91	Straight	5	6	0	3-OOH	2.1457E-10
92	Straight	6	6	0	3-OOH	7.0157E-11
93	Straight	7	6	0	3-OOH	2.2940E-11
94	Straight	8	6	0	3-OOH	7.5007E-12
95	Straight	9	6	0	3-OOH	2.4525E-12
96	Straight	10	6	0	3-OOH	8.0192E-13
97	Straight	11	6	0	3-OOH	2.6221E-13
98	Straight	12	6	0	3-OOH	8.5735E-14
99	Straight	13	6	0	3-OOH	2.8033E-14
100	Straight	14	6	0	3-OOH	9.1662E-15
101	Straight	5	3	1	1-ONO_2	2.7776E-03
102	Straight	6	3	1	1-ONO_2	9.0821E-04
103	Straight	7	3	1	1-ONO_2	2.9696E-04
104	Straight	8	3	1	1-ONO_2	9.7099E-05
105	Straight	9	3	1	1-ONO_2	3.1749E-05
106	Straight	10	3	1	1-ONO_2	1.0381E-05
107	Straight	11	3	1	1-ONO_2	3.3944E-06
108	Straight	12	3	1	1-ONO_2	1.1099E-06
109	Straight	13	3	1	1-ONO_2	3.6290E-07
110	Straight	14	3	1	1-ONO_2	1.1866E-07
111	Straight	5	6	2	2-ONO_2	1.1897E-05
112	Straight	6	6	2	2-ONO_2	3.8901E-06
113	Straight	7	6	2	2-ONO_2	1.2720E-06
114	Straight	8	6	2	2-ONO_2	4.1590E-07
115	Straight	9	6	2	2-ONO_2	1.3599E-07
116	Straight	10	6	2	2-ONO_2	4.4465E-08
117	Straight	11	6	2	2-ONO_2	1.4539E-08
118	Straight	12	6	2	2-ONO_2	4.7538E-09
119	Straight	13	6	2	2-ONO_2	1.5544E-09
120	Straight	14	6	2	2-ONO_2	5.0824E-10
121	Straight	5	9	3	3-ONO_2	5.0958E-08
122	Straight	6	9	3	3-ONO_2	1.6662E-08
123	Straight	7	9	3	3-ONO_2	5.4481E-09
124	Straight	8	9	3	3-ONO_2	1.7814E-09
125	Straight	9	9	3	3-ONO_2	5.8247E-10

126	Straight	10	9	3	3-ONO_2	1.9045E-10
127	Straight	11	9	3	3-ONO_2	6.2273E-11
128	Straight	12	9	3	3-ONO_2	2.0362E-11
129	Straight	13	9	3	3-ONO_2	6.6578E-12
130	Straight	14	9	3	3-ONO_2	2.1769E-12
131	Straight	5	2	0	1-OH+1-C=O	8.3089E-04
132	Straight	6	2	0	1-OH+1-C=O	2.7168E-04
133	Straight	7	2	0	1-OH+1-C=O	8.8832E-05
134	Straight	8	2	0	1-OH+1-C=O	2.9046E-05
135	Straight	9	2	0	1-OH+1-C=O	9.4973E-06
136	Straight	10	2	0	1-OH+1-C=O	3.1054E-06
137	Straight	11	2	0	1-OH+1-C=O	1.0154E-06
138	Straight	12	2	0	1-OH+1-C=O	3.3200E-07
139	Straight	13	2	0	1-OH+1-C=O	1.0856E-07
140	Straight	14	2	0	1-OH+1-C=O	3.5495E-08
141	Straight	5	3	0	1-OH+1-OOH	7.3193E-06
142	Straight	6	3	0	1-OH+1-OOH	2.3932E-06
143	Straight	7	3	0	1-OH+1-OOH	7.8253E-07
144	Straight	8	3	0	1-OH+1-OOH	2.5587E-07
145	Straight	9	3	0	1-OH+1-OOH	8.3662E-08
146	Straight	10	3	0	1-OH+1-OOH	2.7355E-08
147	Straight	11	3	0	1-OH+1-OOH	8.9445E-09
148	Straight	12	3	0	1-OH+1-OOH	2.9246E-09
149	Straight	13	3	0	1-OH+1-OOH	9.5628E-10
150	Straight	14	3	0	1-OH+1-OOH	3.1268E-10
151	Straight	5	4	1	1-OH+1-ONO_2	5.5771E-05
152	Straight	6	4	1	1-OH+1-ONO_2	1.8236E-05
153	Straight	7	4	1	1-OH+1-ONO_2	5.9626E-06
154	Straight	8	4	1	1-OH+1-ONO_2	1.9496E-06
155	Straight	9	4	1	1-OH+1-ONO_2	6.3747E-07
156	Straight	10	4	1	1-OH+1-ONO_2	2.0844E-07
157	Straight	11	4	1	1-OH+1-ONO_2	6.8154E-08
158	Straight	12	4	1	1-OH+1-ONO_2	2.2285E-08
159	Straight	13	4	1	1-OH+1-ONO_2	7.2865E-09
160	Straight	14	4	1	1-OH+1-ONO_2	2.3825E-09
161	Straight	5	3	0	1-C=O+1-OOH	6.1353E-05
162	Straight	6	3	0	1-C=O+1-OOH	2.0061E-05
163	Straight	7	3	0	1-C=O+1-OOH	6.5594E-06
164	Straight	8	3	0	1-C=O+1-OOH	2.1448E-06
165	Straight	9	3	0	1-C=O+1-OOH	7.0128E-07
166	Straight	10	3	0	1-C=O+1-OOH	2.2930E-07
167	Straight	11	3	0	1-C=O+1-OOH	7.4976E-08

168	Straight	12	3	0	1-C=O+1-OOH	2.4515E-08
169	Straight	13	3	0	1-C=O+1-OOH	8.0158E-09
170	Straight	14	3	0	1-C=O+1-OOH	2.6210E-09
171	Straight	5	4	1	1-C=O+1-ONO_2	1.7725E-04
172	Straight	6	4	1	1-C=O+1-ONO_2	5.7956E-05
173	Straight	7	4	1	1-C=O+1-ONO_2	1.8950E-05
174	Straight	8	4	1	1-C=O+1-ONO_2	6.1962E-06
175	Straight	9	4	1	1-C=O+1-ONO_2	2.0260E-06
176	Straight	10	4	1	1-C=O+1-ONO_2	6.6245E-07
177	Straight	11	4	1	1-C=O+1-ONO_2	2.1660E-07
178	Straight	12	4	1	1-C=O+1-ONO_2	7.0824E-08
179	Straight	13	4	1	1-C=O+1-ONO_2	2.3158E-08
180	Straight	14	4	1	1-C=O+1-ONO_2	7.5720E-09
181	Straight	5	5	1	1-OOH+1-ONO_2	4.1181E-06
182	Straight	6	5	1	1-OOH+1-ONO_2	1.3465E-06
183	Straight	7	5	1	1-OOH+1-ONO_2	4.4028E-07
184	Straight	8	5	1	1-OOH+1-ONO_2	1.4396E-07
185	Straight	9	5	1	1-OOH+1-ONO_2	4.7071E-08
186	Straight	10	5	1	1-OOH+1-ONO_2	1.5391E-08
187	Straight	11	5	1	1-OOH+1-ONO_2	5.0325E-09
188	Straight	12	5	1	1-OOH+1-ONO_2	1.6455E-09
189	Straight	13	5	1	1-OOH+1-ONO_2	5.3804E-10
190	Straight	14	5	1	1-OOH+1-ONO_2	1.7592E-10
191	Straight	5	3	0	2-OH+1-C=O	1.6605E-06
192	Straight	6	3	0	2-OH+1-C=O	5.4293E-07
193	Straight	7	3	0	2-OH+1-C=O	1.7752E-07
194	Straight	8	3	0	2-OH+1-C=O	5.8046E-08
195	Straight	9	3	0	2-OH+1-C=O	1.8980E-08
196	Straight	10	3	0	2-OH+1-C=O	6.2058E-09
197	Straight	11	3	0	2-OH+1-C=O	2.0292E-09
198	Straight	12	3	0	2-OH+1-C=O	6.6348E-10
199	Straight	13	3	0	2-OH+1-C=O	2.1694E-10
200	Straight	14	3	0	2-OH+1-C=O	7.0935E-11
201	Straight	5	4	0	2-OH+1-OOH	1.1194E-08
202	Straight	6	4	0	2-OH+1-OOH	3.6603E-09
203	Straight	7	4	0	2-OH+1-OOH	1.1968E-09
204	Straight	8	4	0	2-OH+1-OOH	3.9133E-10
205	Straight	9	4	0	2-OH+1-OOH	1.2795E-10
206	Straight	10	4	0	2-OH+1-OOH	4.1838E-11
207	Straight	11	4	0	2-OH+1-OOH	1.3680E-11
208	Straight	12	4	0	2-OH+1-OOH	4.4730E-12

209	Straight	13	4	0	2-OH+1-OOH	1.4626E-12
210	Straight	14	4	0	2-OH+1-OOH	4.7822E-13
211	Straight	5	5	1	2-OH+1-ONO_2	1.1145E-07
212	Straight	6	5	1	2-OH+1-ONO_2	3.6442E-08
213	Straight	7	5	1	2-OH+1-ONO_2	1.1916E-08
214	Straight	8	5	1	2-OH+1-ONO_2	3.8961E-09
215	Straight	9	5	1	2-OH+1-ONO_2	1.2739E-09
216	Straight	10	5	1	2-OH+1-ONO_2	4.1655E-10
217	Straight	11	5	1	2-OH+1-ONO_2	1.3620E-10
218	Straight	12	5	1	2-OH+1-ONO_2	4.4534E-11
219	Straight	13	5	1	2-OH+1-ONO_2	1.4561E-11
220	Straight	14	5	1	2-OH+1-ONO_2	4.7612E-12
221	Straight	5	3	0	2-C=O+1-OH	1.3683E-04
222	Straight	6	3	0	2-C=O+1-OH	4.4739E-05
223	Straight	7	3	0	2-C=O+1-OH	1.4629E-05
224	Straight	8	3	0	2-C=O+1-OH	4.7832E-06
225	Straight	9	3	0	2-C=O+1-OH	1.5640E-06
226	Straight	10	3	0	2-C=O+1-OH	5.1138E-07
227	Straight	11	3	0	2-C=O+1-OH	1.6721E-07
228	Straight	12	3	0	2-C=O+1-OH	5.4673E-08
229	Straight	13	3	0	2-C=O+1-OH	1.7877E-08
230	Straight	14	3	0	2-C=O+1-OH	5.8452E-09
231	Straight	5	4	0	2-C=O+1-OOH	1.0103E-05
232	Straight	6	4	0	2-C=O+1-OOH	3.3035E-06
233	Straight	7	4	0	2-C=O+1-OOH	1.0802E-06
234	Straight	8	4	0	2-C=O+1-OOH	3.5319E-07
235	Straight	9	4	0	2-C=O+1-OOH	1.1548E-07
236	Straight	10	4	0	2-C=O+1-OOH	3.7760E-08
237	Straight	11	4	0	2-C=O+1-OOH	1.2347E-08
238	Straight	12	4	0	2-C=O+1-OOH	4.0371E-09
239	Straight	13	4	0	2-C=O+1-OOH	1.3200E-09
240	Straight	14	4	0	2-C=O+1-OOH	4.3161E-10
241	Straight	5	5	1	2-C=O+1-ONO_2	2.9189E-05
242	Straight	6	5	1	2-C=O+1-ONO_2	9.5439E-06
243	Straight	7	5	1	2-C=O+1-ONO_2	3.1206E-06
244	Straight	8	5	1	2-C=O+1-ONO_2	1.0204E-06
245	Straight	9	5	1	2-C=O+1-ONO_2	3.3363E-07
246	Straight	10	5	1	2-C=O+1-ONO_2	1.0909E-07
247	Straight	11	5	1	2-C=O+1-ONO_2	3.5670E-08
248	Straight	12	5	1	2-C=O+1-ONO_2	1.1663E-08
249	Straight	13	5	1	2-C=O+1-ONO_2	3.8135E-09

250	Straight	14	5	1	2-C=O+1-ONO_2	1.2469E-09
251	Straight	5	5	0	2-OOH+1-OH	3.2943E-09
252	Straight	6	5	0	2-OOH+1-OH	1.0772E-09
253	Straight	7	5	0	2-OOH+1-OH	3.5220E-10
254	Straight	8	5	0	2-OOH+1-OH	1.1516E-10
255	Straight	9	5	0	2-OOH+1-OH	3.7655E-11
256	Straight	10	5	0	2-OOH+1-OH	1.2312E-11
257	Straight	11	5	0	2-OOH+1-OH	4.0258E-12
258	Straight	12	5	0	2-OOH+1-OH	1.3163E-12
259	Straight	13	5	0	2-OOH+1-OH	4.3041E-13
260	Straight	14	5	0	2-OOH+1-OH	1.4073E-13
261	Straight	5	5	0	2-OOH+1-C=O	3.1616E-08
262	Straight	6	5	0	2-OOH+1-C=O	1.0338E-08
263	Straight	7	5	0	2-OOH+1-C=O	3.3801E-09
264	Straight	8	5	0	2-OOH+1-C=O	1.1052E-09
265	Straight	9	5	0	2-OOH+1-C=O	3.6138E-10
266	Straight	10	5	0	2-OOH+1-C=O	1.1816E-10
267	Straight	11	5	0	2-OOH+1-C=O	3.8636E-11
268	Straight	12	5	0	2-OOH+1-C=O	1.2633E-11
269	Straight	13	5	0	2-OOH+1-C=O	4.1307E-12
270	Straight	14	5	0	2-OOH+1-C=O	1.3506E-12
271	Straight	5	7	1	2-OOH+1-ONO_2	2.1221E-09
272	Straight	6	7	1	2-OOH+1-ONO_2	6.9388E-10
273	Straight	7	7	1	2-OOH+1-ONO_2	2.2688E-10
274	Straight	8	7	1	2-OOH+1-ONO_2	7.4184E-11
275	Straight	9	7	1	2-OOH+1-ONO_2	2.4256E-11
276	Straight	10	7	1	2-OOH+1-ONO_2	7.9312E-12
277	Straight	11	7	1	2-OOH+1-ONO_2	2.5933E-12
278	Straight	12	7	1	2-OOH+1-ONO_2	8.4795E-13
279	Straight	13	7	1	2-OOH+1-ONO_2	2.7726E-13
280	Straight	14	7	1	2-OOH+1-ONO_2	9.0656E-14
281	Straight	5	7	2	2-ONO_2+1-OH	2.3888E-07
282	Straight	6	7	2	2-ONO_2+1-OH	7.8107E-08
283	Straight	7	7	2	2-ONO_2+1-OH	2.5539E-08
284	Straight	8	7	2	2-ONO_2+1-OH	8.3506E-09
285	Straight	9	7	2	2-ONO_2+1-OH	2.7304E-09
286	Straight	10	7	2	2-ONO_2+1-OH	8.9278E-10
287	Straight	11	7	2	2-ONO_2+1-OH	2.9192E-10
288	Straight	12	7	2	2-ONO_2+1-OH	9.5450E-11
289	Straight	13	7	2	2-ONO_2+1-OH	3.1210E-11
290	Straight	14	7	2	2-ONO_2+1-OH	1.0205E-11

291	Straight	5	7	2	2-ONO_2+1-C=O	7.5919E-07
292	Straight	6	7	2	2-ONO_2+1-C=O	2.4824E-07
293	Straight	7	7	2	2-ONO_2+1-C=O	8.1167E-08
294	Straight	8	7	2	2-ONO_2+1-C=O	2.6540E-08
295	Straight	9	7	2	2-ONO_2+1-C=O	8.6778E-09
296	Straight	10	7	2	2-ONO_2+1-C=O	2.8374E-09
297	Straight	11	7	2	2-ONO_2+1-C=O	9.2777E-10
298	Straight	12	7	2	2-ONO_2+1-C=O	3.0336E-10
299	Straight	13	7	2	2-ONO_2+1-C=O	9.9190E-11
300	Straight	14	7	2	2-ONO_2+1-C=O	3.2433E-11
301	Straight	5	8	2	2-ONO_2+1-OOH	1.7639E-08
302	Straight	6	8	2	2-ONO_2+1-OOH	5.7674E-09
303	Straight	7	8	2	2-ONO_2+1-OOH	1.8858E-09
304	Straight	8	8	2	2-ONO_2+1-OOH	6.1661E-10
305	Straight	9	8	2	2-ONO_2+1-OOH	2.0162E-10
306	Straight	10	8	2	2-ONO_2+1-OOH	6.5923E-11
307	Straight	11	8	2	2-ONO_2+1-OOH	2.1555E-11
308	Straight	12	8	2	2-ONO_2+1-OOH	7.0480E-12
309	Straight	13	8	2	2-ONO_2+1-OOH	2.3045E-12
310	Straight	14	8	2	2-ONO_2+1-OOH	7.5352E-13
311	Straight	5	4	0	1-OH+1-C=O+1-OOH	4.6707E-07
312	Straight	6	4	0	1-OH+1-C=O+1-OOH	1.5272E-07
313	Straight	7	4	0	1-OH+1-C=O+1-OOH	4.9936E-08
314	Straight	8	4	0	1-OH+1-C=O+1-OOH	1.6328E-08
315	Straight	9	4	0	1-OH+1-C=O+1-OOH	5.3387E-09
316	Straight	10	4	0	1-OH+1-C=O+1-OOH	1.7456E-09
317	Straight	11	4	0	1-OH+1-C=O+1-OOH	5.7078E-10
318	Straight	12	4	0	1-OH+1-C=O+1-OOH	1.8663E-10
319	Straight	13	4	0	1-OH+1-C=O+1-OOH	6.1023E-11
320	Straight	14	4	0	1-OH+1-C=O+1-OOH	1.9953E-11
321	Straight	5	5	1	1-OH+1-C=O+1-ONO_2	3.5589E-06
322	Straight	6	5	1	1-OH+1-C=O+1-ONO_2	1.1637E-06
323	Straight	7	5	1	1-OH+1-C=O+1-ONO_2	3.8049E-07
324	Straight	8	5	1	1-OH+1-C=O+1-ONO_2	1.2441E-07
325	Straight	9	5	1	1-OH+1-C=O+1-ONO_2	4.0679E-08
326	Straight	10	5	1	1-OH+1-C=O+1-ONO_2	1.3301E-08
327	Straight	11	5	1	1-OH+1-C=O+1-ONO_2	4.3491E-09
328	Straight	12	5	1	1-OH+1-C=O+1-ONO_2	1.4220E-09
329	Straight	13	5	1	1-OH+1-C=O+1-ONO_2	4.6497E-10
330	Straight	14	5	1	1-OH+1-C=O+1-ONO_2	1.5203E-10

331	Straight	5	6	1	1-OH+1-OOH+1-ONO_2	3.1350E-08
332	Straight	6	6	1	1-OH+1-OOH+1-ONO_2	1.0251E-08
333	Straight	7	6	1	1-OH+1-OOH+1-ONO_2	3.3518E-09
334	Straight	8	6	1	1-OH+1-OOH+1-ONO_2	1.0959E-09
335	Straight	9	6	1	1-OH+1-OOH+1-ONO_2	3.5834E-10
336	Straight	10	6	1	1-OH+1-OOH+1-ONO_2	1.1717E-10
337	Straight	11	6	1	1-OH+1-OOH+1-ONO_2	3.8311E-11
338	Straight	12	6	1	1-OH+1-OOH+1-ONO_2	1.2527E-11
339	Straight	13	6	1	1-OH+1-OOH+1-ONO_2	4.0960E-12
340	Straight	14	6	1	1-OH+1-OOH+1-ONO_2	1.3393E-12
341	Straight	5	6	1	1-C=O+1-OOH+1-ONO_2	2.6279E-07
342	Straight	6	6	1	1-C=O+1-OOH+1-ONO_2	8.5925E-08
343	Straight	7	6	1	1-C=O+1-OOH+1-ONO_2	2.8095E-08
344	Straight	8	6	1	1-C=O+1-OOH+1-ONO_2	9.1865E-09
345	Straight	9	6	1	1-C=O+1-OOH+1-ONO_2	3.0037E-09
346	Straight	10	6	1	1-C=O+1-OOH+1-ONO_2	9.8215E-10
347	Straight	11	6	1	1-C=O+1-OOH+1-ONO_2	3.2114E-10
348	Straight	12	6	1	1-C=O+1-OOH+1-ONO_2	1.0500E-10
349	Straight	13	6	1	1-C=O+1-OOH+1-ONO_2	3.4334E-11
350	Straight	14	6	1	1-C=O+1-OOH+1-ONO_2	1.1226E-11
351	Straight	5	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	2.0006E-09
352	Straight	6	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	6.5413E-10
353	Straight	7	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	2.1389E-10
354	Straight	8	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	6.9935E-11
355	Straight	9	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	2.2867E-11
356	Straight	10	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	7.4769E-12
357	Straight	11	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	2.4448E-12
358	Straight	12	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	7.9938E-13
359	Straight	13	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	2.6138E-13
360	Straight	14	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	8.5463E-14
361	Branching	5	0	0	-	1.0263E+00
362	Branching	6	0	0	-	3.3557E-01
363	Branching	7	0	0	-	1.0972E-01
364	Branching	8	0	0	-	3.5877E-02
365	Branching	9	0	0	-	1.1731E-02
366	Branching	10	0	0	-	3.8357E-03
367	Branching	11	0	0	-	1.2542E-03
368	Branching	12	0	0	-	4.1008E-04
369	Branching	13	0	0	-	1.3409E-04
370	Branching	14	0	0	-	4.3843E-05

371	Branching	5	1	0	1-OH	2.0607E-02
372	Branching	6	1	0	1-OH	6.7378E-03
373	Branching	7	1	0	1-OH	2.2031E-03
374	Branching	8	1	0	1-OH	7.2036E-04
375	Branching	9	1	0	1-OH	2.3554E-04
376	Branching	10	1	0	1-OH	7.7015E-05
377	Branching	11	1	0	1-OH	2.5182E-05
378	Branching	12	1	0	1-OH	8.2339E-06
379	Branching	13	1	0	1-OH	2.6923E-06
380	Branching	14	1	0	1-OH	8.8030E-07
381	Branching	5	2	0	2-OH	4.7622E-05
382	Branching	6	2	0	2-OH	1.5571E-05
383	Branching	7	2	0	2-OH	5.0914E-06
384	Branching	8	2	0	2-OH	1.6648E-06
385	Branching	9	2	0	2-OH	5.4434E-07
386	Branching	10	2	0	2-OH	1.7798E-07
387	Branching	11	2	0	2-OH	5.8197E-08
388	Branching	12	2	0	2-OH	1.9029E-08
389	Branching	13	2	0	2-OH	6.2219E-09
390	Branching	14	2	0	2-OH	2.0344E-09
391	Branching	5	3	0	3-OH	8.1511E-08
392	Branching	6	3	0	3-OH	2.6652E-08
393	Branching	7	3	0	3-OH	8.7146E-09
394	Branching	8	3	0	3-OH	2.8494E-09
395	Branching	9	3	0	3-OH	9.3170E-10
396	Branching	10	3	0	3-OH	3.0464E-10
397	Branching	11	3	0	3-OH	9.9610E-11
398	Branching	12	3	0	3-OH	3.2570E-11
399	Branching	13	3	0	3-OH	1.0650E-11
400	Branching	14	3	0	3-OH	3.4821E-12
401	Branching	5	1	0	1-C=O	6.5491E-02
402	Branching	6	1	0	1-C=O	2.1414E-02
403	Branching	7	1	0	1-C=O	7.0018E-03
404	Branching	8	1	0	1-C=O	2.2894E-03
405	Branching	9	1	0	1-C=O	7.4858E-04
406	Branching	10	1	0	1-C=O	2.4477E-04
407	Branching	11	1	0	1-C=O	8.0033E-05
408	Branching	12	1	0	1-C=O	2.6169E-05
409	Branching	13	1	0	1-C=O	8.5565E-06
410	Branching	14	1	0	1-C=O	2.7978E-06
411	Branching	5	2	0	2-C=O	5.9400E-03
412	Branching	6	2	0	2-C=O	1.9422E-03
413	Branching	7	2	0	2-C=O	6.3506E-04
414	Branching	8	2	0	2-C=O	2.0765E-04

415	Branching	9	2	0	2-C=O	6.7896E-05
416	Branching	10	2	0	2-C=O	2.2200E-05
417	Branching	11	2	0	2-C=O	7.2589E-06
418	Branching	12	2	0	2-C=O	2.3735E-06
419	Branching	13	2	0	2-C=O	7.7607E-07
420	Branching	14	2	0	2-C=O	2.5375E-07
421	Branching	5	3	0	3-C=O	7.8049E-04
422	Branching	6	3	0	3-C=O	2.5520E-04
423	Branching	7	3	0	3-C=O	8.3444E-05
424	Branching	8	3	0	3-C=O	2.7284E-05
425	Branching	9	3	0	3-C=O	8.9213E-06
426	Branching	10	3	0	3-C=O	2.9170E-06
427	Branching	11	3	0	3-C=O	9.5379E-07
428	Branching	12	3	0	3-C=O	3.1187E-07
429	Branching	13	3	0	3-C=O	1.0197E-07
430	Branching	14	3	0	3-C=O	3.3342E-08
431	Branching	5	2	0	1-OOH	1.5216E-03
432	Branching	6	2	0	1-OOH	4.9752E-04
433	Branching	7	2	0	1-OOH	1.6268E-04
434	Branching	8	2	0	1-OOH	5.3191E-05
435	Branching	9	2	0	1-OOH	1.7392E-05
436	Branching	10	2	0	1-OOH	5.6868E-06
437	Branching	11	2	0	1-OOH	1.8594E-06
438	Branching	12	2	0	1-OOH	6.0799E-07
439	Branching	13	2	0	1-OOH	1.9880E-07
440	Branching	14	2	0	1-OOH	6.5002E-08
441	Branching	5	4	0	2-OOH	7.8409E-07
442	Branching	6	4	0	2-OOH	2.5638E-07
443	Branching	7	4	0	2-OOH	8.3829E-08
444	Branching	8	4	0	2-OOH	2.7410E-08
445	Branching	9	4	0	2-OOH	8.9624E-09
446	Branching	10	4	0	2-OOH	2.9305E-09
447	Branching	11	4	0	2-OOH	9.5819E-10
448	Branching	12	4	0	2-OOH	3.1331E-10
449	Branching	13	4	0	2-OOH	1.0244E-10
450	Branching	14	4	0	2-OOH	3.3496E-11
451	Branching	5	6	0	3-OOH	3.3957E-10
452	Branching	6	6	0	3-OOH	1.1103E-10
453	Branching	7	6	0	3-OOH	3.6304E-11
454	Branching	8	6	0	3-OOH	1.1871E-11
455	Branching	9	6	0	3-OOH	3.8814E-12
456	Branching	10	6	0	3-OOH	1.2691E-12
457	Branching	11	6	0	3-OOH	4.1497E-13
458	Branching	12	6	0	3-OOH	1.3568E-13

459	Branching	13	6	0	3-OOH	4.4365E-14
460	Branching	14	6	0	3-OOH	1.4506E-14
461	Branching	5	3	1	1-ONO_2	4.3959E-03
462	Branching	6	3	1	1-ONO_2	1.4373E-03
463	Branching	7	3	1	1-ONO_2	4.6997E-04
464	Branching	8	3	1	1-ONO_2	1.5367E-04
465	Branching	9	3	1	1-ONO_2	5.0246E-05
466	Branching	10	3	1	1-ONO_2	1.6429E-05
467	Branching	11	3	1	1-ONO_2	5.3719E-06
468	Branching	12	3	1	1-ONO_2	1.7565E-06
469	Branching	13	3	1	1-ONO_2	5.7433E-07
470	Branching	14	3	1	1-ONO_2	1.8779E-07
471	Branching	5	6	2	2-ONO_2	1.8828E-05
472	Branching	6	6	2	2-ONO_2	6.1564E-06
473	Branching	7	6	2	2-ONO_2	2.0130E-06
474	Branching	8	6	2	2-ONO_2	6.5820E-07
475	Branching	9	6	2	2-ONO_2	2.1521E-07
476	Branching	10	6	2	2-ONO_2	7.0370E-08
477	Branching	11	6	2	2-ONO_2	2.3009E-08
478	Branching	12	6	2	2-ONO_2	7.5234E-09
479	Branching	13	6	2	2-ONO_2	2.4600E-09
480	Branching	14	6	2	2-ONO_2	8.0435E-10
481	Branching	5	9	3	3-ONO_2	8.0646E-08
482	Branching	6	9	3	3-ONO_2	2.6369E-08
483	Branching	7	9	3	3-ONO_2	8.6221E-09
484	Branching	8	9	3	3-ONO_2	2.8192E-09
485	Branching	9	9	3	3-ONO_2	9.2181E-10
486	Branching	10	9	3	3-ONO_2	3.0141E-10
487	Branching	11	9	3	3-ONO_2	9.8553E-11
488	Branching	12	9	3	3-ONO_2	3.2224E-11
489	Branching	13	9	3	3-ONO_2	1.0537E-11
490	Branching	14	9	3	3-ONO_2	3.4452E-12
491	Branching	5	2	0	1-OH+1-C=O	1.3150E-03
492	Branching	6	2	0	1-OH+1-C=O	4.2996E-04
493	Branching	7	2	0	1-OH+1-C=O	1.4059E-04
494	Branching	8	2	0	1-OH+1-C=O	4.5968E-05
495	Branching	9	2	0	1-OH+1-C=O	1.5030E-05
496	Branching	10	2	0	1-OH+1-C=O	4.9146E-06
497	Branching	11	2	0	1-OH+1-C=O	1.6069E-06
498	Branching	12	2	0	1-OH+1-C=O	5.2543E-07

499	Branching	13	2	0	1-OH+1-C=O	1.7180E-07
500	Branching	14	2	0	1-OH+1-C=O	5.6175E-08
501	Branching	5	3	0	1-OH+1-OOH	1.1584E-05
502	Branching	6	3	0	1-OH+1-OOH	3.7875E-06
503	Branching	7	3	0	1-OH+1-OOH	1.2384E-06
504	Branching	8	3	0	1-OH+1-OOH	4.0494E-07
505	Branching	9	3	0	1-OH+1-OOH	1.3240E-07
506	Branching	10	3	0	1-OH+1-OOH	4.3293E-08
507	Branching	11	3	0	1-OH+1-OOH	1.4156E-08
508	Branching	12	3	0	1-OH+1-OOH	4.6285E-09
509	Branching	13	3	0	1-OH+1-OOH	1.5134E-09
510	Branching	14	3	0	1-OH+1-OOH	4.9485E-10
511	Branching	5	4	1	1-OH+1-ONO_2	8.8262E-05
512	Branching	6	4	1	1-OH+1-ONO_2	2.8860E-05
513	Branching	7	4	1	1-OH+1-ONO_2	9.4363E-06
514	Branching	8	4	1	1-OH+1-ONO_2	3.0854E-06
515	Branching	9	4	1	1-OH+1-ONO_2	1.0089E-06
516	Branching	10	4	1	1-OH+1-ONO_2	3.2987E-07
517	Branching	11	4	1	1-OH+1-ONO_2	1.0786E-07
518	Branching	12	4	1	1-OH+1-ONO_2	3.5268E-08
519	Branching	13	4	1	1-OH+1-ONO_2	1.1532E-08
520	Branching	14	4	1	1-OH+1-ONO_2	3.7705E-09
521	Branching	5	3	0	1-C=O+1-OOH	9.7097E-05
522	Branching	6	3	0	1-C=O+1-OOH	3.1748E-05
523	Branching	7	3	0	1-C=O+1-OOH	1.0381E-05
524	Branching	8	3	0	1-C=O+1-OOH	3.3943E-06
525	Branching	9	3	0	1-C=O+1-OOH	1.1098E-06
526	Branching	10	3	0	1-C=O+1-OOH	3.6289E-07
527	Branching	11	3	0	1-C=O+1-OOH	1.1866E-07
528	Branching	12	3	0	1-C=O+1-OOH	3.8798E-08
529	Branching	13	3	0	1-C=O+1-OOH	1.2686E-08
530	Branching	14	3	0	1-C=O+1-OOH	4.1480E-09
531	Branching	5	4	1	1-C=O+1-ONO_2	2.8051E-04
532	Branching	6	4	1	1-C=O+1-ONO_2	9.1721E-05
533	Branching	7	4	1	1-C=O+1-ONO_2	2.9990E-05
534	Branching	8	4	1	1-C=O+1-ONO_2	9.8061E-06
535	Branching	9	4	1	1-C=O+1-ONO_2	3.2063E-06
536	Branching	10	4	1	1-C=O+1-ONO_2	1.0484E-06
537	Branching	11	4	1	1-C=O+1-ONO_2	3.4280E-07
538	Branching	12	4	1	1-C=O+1-ONO_2	1.1209E-07
539	Branching	13	4	1	1-C=O+1-ONO_2	3.6649E-08

540	Branching	14	4	1	1-C=O+1-ONO_2	1.1983E-08
541	Branching	5	5	1	1-OOH+1-ONO_2	6.5173E-06
542	Branching	6	5	1	1-OOH+1-ONO_2	2.1310E-06
543	Branching	7	5	1	1-OOH+1-ONO_2	6.9678E-07
544	Branching	8	5	1	1-OOH+1-ONO_2	2.2783E-07
545	Branching	9	5	1	1-OOH+1-ONO_2	7.4494E-08
546	Branching	10	5	1	1-OOH+1-ONO_2	2.4358E-08
547	Branching	11	5	1	1-OOH+1-ONO_2	7.9644E-09
548	Branching	12	5	1	1-OOH+1-ONO_2	2.6042E-09
549	Branching	13	5	1	1-OOH+1-ONO_2	8.5149E-10
550	Branching	14	5	1	1-OOH+1-ONO_2	2.7842E-10
551	Branching	5	3	0	2-OH+1-C=O	2.6278E-06
552	Branching	6	3	0	2-OH+1-C=O	8.5924E-07
553	Branching	7	3	0	2-OH+1-C=O	2.8095E-07
554	Branching	8	3	0	2-OH+1-C=O	9.1864E-08
555	Branching	9	3	0	2-OH+1-C=O	3.0037E-08
556	Branching	10	3	0	2-OH+1-C=O	9.8214E-09
557	Branching	11	3	0	2-OH+1-C=O	3.2113E-09
558	Branching	12	3	0	2-OH+1-C=O	1.0500E-09
559	Branching	13	3	0	2-OH+1-C=O	3.4333E-10
560	Branching	14	3	0	2-OH+1-C=O	1.1226E-10
561	Branching	5	4	0	2-OH+1-OOH	1.7716E-08
562	Branching	6	4	0	2-OH+1-OOH	5.7927E-09
563	Branching	7	4	0	2-OH+1-OOH	1.8941E-09
564	Branching	8	4	0	2-OH+1-OOH	6.1932E-10
565	Branching	9	4	0	2-OH+1-OOH	2.0250E-10
566	Branching	10	4	0	2-OH+1-OOH	6.6213E-11
567	Branching	11	4	0	2-OH+1-OOH	2.1650E-11
568	Branching	12	4	0	2-OH+1-OOH	7.0790E-12
569	Branching	13	4	0	2-OH+1-OOH	2.3146E-12
570	Branching	14	4	0	2-OH+1-OOH	7.5683E-13
571	Branching	5	5	1	2-OH+1-ONO_2	1.7639E-07
572	Branching	6	5	1	2-OH+1-ONO_2	5.7674E-08
573	Branching	7	5	1	2-OH+1-ONO_2	1.8858E-08
574	Branching	8	5	1	2-OH+1-ONO_2	6.1660E-09
575	Branching	9	5	1	2-OH+1-ONO_2	2.0161E-09
576	Branching	10	5	1	2-OH+1-ONO_2	6.5922E-10
577	Branching	11	5	1	2-OH+1-ONO_2	2.1555E-10
578	Branching	12	5	1	2-OH+1-ONO_2	7.0479E-11
579	Branching	13	5	1	2-OH+1-ONO_2	2.3045E-11
580	Branching	14	5	1	2-OH+1-ONO_2	7.5351E-12

581	Branching	5	3	0	2-C=O+1-OH	2.1654E-04
582	Branching	6	3	0	2-C=O+1-OH	7.0804E-05
583	Branching	7	3	0	2-C=O+1-OH	2.3151E-05
584	Branching	8	3	0	2-C=O+1-OH	7.5699E-06
585	Branching	9	3	0	2-C=O+1-OH	2.4752E-06
586	Branching	10	3	0	2-C=O+1-OH	8.0931E-07
587	Branching	11	3	0	2-C=O+1-OH	2.6462E-07
588	Branching	12	3	0	2-C=O+1-OH	8.6526E-08
589	Branching	13	3	0	2-C=O+1-OH	2.8292E-08
590	Branching	14	3	0	2-C=O+1-OH	9.2507E-09
591	Branching	5	4	0	2-C=O+1-OOH	1.5990E-05
592	Branching	6	4	0	2-C=O+1-OOH	5.2282E-06
593	Branching	7	4	0	2-C=O+1-OOH	1.7095E-06
594	Branching	8	4	0	2-C=O+1-OOH	5.5896E-07
595	Branching	9	4	0	2-C=O+1-OOH	1.8277E-07
596	Branching	10	4	0	2-C=O+1-OOH	5.9760E-08
597	Branching	11	4	0	2-C=O+1-OOH	1.9540E-08
598	Branching	12	4	0	2-C=O+1-OOH	6.3891E-09
599	Branching	13	4	0	2-C=O+1-OOH	2.0891E-09
600	Branching	14	4	0	2-C=O+1-OOH	6.8307E-10
601	Branching	5	5	1	2-C=O+1-ONO_2	4.6194E-05
602	Branching	6	5	1	2-C=O+1-ONO_2	1.5104E-05
603	Branching	7	5	1	2-C=O+1-ONO_2	4.9387E-06
604	Branching	8	5	1	2-C=O+1-ONO_2	1.6148E-06
605	Branching	9	5	1	2-C=O+1-ONO_2	5.2801E-07
606	Branching	10	5	1	2-C=O+1-ONO_2	1.7265E-07
607	Branching	11	5	1	2-C=O+1-ONO_2	5.6451E-08
608	Branching	12	5	1	2-C=O+1-ONO_2	1.8458E-08
609	Branching	13	5	1	2-C=O+1-ONO_2	6.0353E-09
610	Branching	14	5	1	2-C=O+1-ONO_2	1.9734E-09
611	Branching	5	5	0	2-OOH+1-OH	5.2136E-09
612	Branching	6	5	0	2-OOH+1-OH	1.7047E-09
613	Branching	7	5	0	2-OOH+1-OH	5.5740E-10
614	Branching	8	5	0	2-OOH+1-OH	1.8226E-10
615	Branching	9	5	0	2-OOH+1-OH	5.9593E-11
616	Branching	10	5	0	2-OOH+1-OH	1.9485E-11
617	Branching	11	5	0	2-OOH+1-OH	6.3712E-12
618	Branching	12	5	0	2-OOH+1-OH	2.0832E-12
619	Branching	13	5	0	2-OOH+1-OH	6.8116E-13
620	Branching	14	5	0	2-OOH+1-OH	2.2272E-13
621	Branching	5	5	0	2-OOH+1-C=O	5.0035E-08
622	Branching	6	5	0	2-OOH+1-C=O	1.6360E-08

623	Branching	7	5	0	2-OOH+1-C=O	5.3494E-09
624	Branching	8	5	0	2-OOH+1-C=O	1.7491E-09
625	Branching	9	5	0	2-OOH+1-C=O	5.7192E-10
626	Branching	10	5	0	2-OOH+1-C=O	1.8700E-10
627	Branching	11	5	0	2-OOH+1-C=O	6.1145E-11
628	Branching	12	5	0	2-OOH+1-C=O	1.9993E-11
629	Branching	13	5	0	2-OOH+1-C=O	6.5372E-12
630	Branching	14	5	0	2-OOH+1-C=O	2.1375E-12
631	Branching	5	7	1	2-OOH+1-ONO_2	3.3584E-09
632	Branching	6	7	1	2-OOH+1-ONO_2	1.0981E-09
633	Branching	7	7	1	2-OOH+1-ONO_2	3.5906E-10
634	Branching	8	7	1	2-OOH+1-ONO_2	1.1740E-10
635	Branching	9	7	1	2-OOH+1-ONO_2	3.8388E-11
636	Branching	10	7	1	2-OOH+1-ONO_2	1.2552E-11
637	Branching	11	7	1	2-OOH+1-ONO_2	4.1042E-12
638	Branching	12	7	1	2-OOH+1-ONO_2	1.3420E-12
639	Branching	13	7	1	2-OOH+1-ONO_2	4.3879E-13
640	Branching	14	7	1	2-OOH+1-ONO_2	1.4347E-13
641	Branching	5	7	2	2-ONO_2+1-OH	3.7805E-07
642	Branching	6	7	2	2-ONO_2+1-OH	1.2361E-07
643	Branching	7	7	2	2-ONO_2+1-OH	4.0418E-08
644	Branching	8	7	2	2-ONO_2+1-OH	1.3216E-08
645	Branching	9	7	2	2-ONO_2+1-OH	4.3212E-09
646	Branching	10	7	2	2-ONO_2+1-OH	1.4129E-09
647	Branching	11	7	2	2-ONO_2+1-OH	4.6199E-10
648	Branching	12	7	2	2-ONO_2+1-OH	1.5106E-10
649	Branching	13	7	2	2-ONO_2+1-OH	4.9392E-11
650	Branching	14	7	2	2-ONO_2+1-OH	1.6150E-11
651	Branching	5	7	2	2-ONO_2+1-C=O	1.2015E-06
652	Branching	6	7	2	2-ONO_2+1-C=O	3.9286E-07
653	Branching	7	7	2	2-ONO_2+1-C=O	1.2846E-07
654	Branching	8	7	2	2-ONO_2+1-C=O	4.2002E-08
655	Branching	9	7	2	2-ONO_2+1-C=O	1.3733E-08
656	Branching	10	7	2	2-ONO_2+1-C=O	4.4905E-09
657	Branching	11	7	2	2-ONO_2+1-C=O	1.4683E-09
658	Branching	12	7	2	2-ONO_2+1-C=O	4.8009E-10
659	Branching	13	7	2	2-ONO_2+1-C=O	1.5698E-10
660	Branching	14	7	2	2-ONO_2+1-C=O	5.1328E-11
661	Branching	5	8	2	2-ONO_2+1-OOH	2.7915E-08
662	Branching	6	8	2	2-ONO_2+1-OOH	9.1275E-09

663	Branching	7	8	2	2-ONO_2+1-OOH	2.9845E-09
664	Branching	8	8	2	2-ONO_2+1-OOH	9.7584E-10
665	Branching	9	8	2	2-ONO_2+1-OOH	3.1908E-10
666	Branching	10	8	2	2-ONO_2+1-OOH	1.0433E-10
667	Branching	11	8	2	2-ONO_2+1-OOH	3.4113E-11
668	Branching	12	8	2	2-ONO_2+1-OOH	1.1154E-11
669	Branching	13	8	2	2-ONO_2+1-OOH	3.6471E-12
670	Branching	14	8	2	2-ONO_2+1-OOH	1.1925E-12
671	Branching	5	4	0	1-OH+1-C=O+1-OOH	7.3918E-07
672	Branching	6	4	0	1-OH+1-C=O+1-OOH	2.4169E-07
673	Branching	7	4	0	1-OH+1-C=O+1-OOH	7.9028E-08
674	Branching	8	4	0	1-OH+1-C=O+1-OOH	2.5840E-08
675	Branching	9	4	0	1-OH+1-C=O+1-OOH	8.4491E-09
676	Branching	10	4	0	1-OH+1-C=O+1-OOH	2.7626E-09
677	Branching	11	4	0	1-OH+1-C=O+1-OOH	9.0331E-10
678	Branching	12	4	0	1-OH+1-C=O+1-OOH	2.9536E-10
679	Branching	13	4	0	1-OH+1-C=O+1-OOH	9.6575E-11
680	Branching	14	4	0	1-OH+1-C=O+1-OOH	3.1578E-11
681	Branching	5	5	1	1-OH+1-C=O+1-ONO_2	5.6323E-06
682	Branching	6	5	1	1-OH+1-C=O+1-ONO_2	1.8416E-06
683	Branching	7	5	1	1-OH+1-C=O+1-ONO_2	6.0216E-07
684	Branching	8	5	1	1-OH+1-C=O+1-ONO_2	1.9689E-07
685	Branching	9	5	1	1-OH+1-C=O+1-ONO_2	6.4379E-08
686	Branching	10	5	1	1-OH+1-C=O+1-ONO_2	2.1050E-08
687	Branching	11	5	1	1-OH+1-C=O+1-ONO_2	6.8829E-09
688	Branching	12	5	1	1-OH+1-C=O+1-ONO_2	2.2505E-09
689	Branching	13	5	1	1-OH+1-C=O+1-ONO_2	7.3587E-10
690	Branching	14	5	1	1-OH+1-C=O+1-ONO_2	2.4061E-10
691	Branching	5	6	1	1-OH+1-OOH+1-ONO_2	4.9615E-08
692	Branching	6	6	1	1-OH+1-OOH+1-ONO_2	1.6223E-08
693	Branching	7	6	1	1-OH+1-OOH+1-ONO_2	5.3045E-09
694	Branching	8	6	1	1-OH+1-OOH+1-ONO_2	1.7344E-09
695	Branching	9	6	1	1-OH+1-OOH+1-ONO_2	5.6711E-10
696	Branching	10	6	1	1-OH+1-OOH+1-ONO_2	1.8543E-10
697	Branching	11	6	1	1-OH+1-OOH+1-ONO_2	6.0632E-11
698	Branching	12	6	1	1-OH+1-OOH+1-ONO_2	1.9825E-11
699	Branching	13	6	1	1-OH+1-OOH+1-ONO_2	6.4823E-12
700	Branching	14	6	1	1-OH+1-OOH+1-ONO_2	2.1195E-12
701	Branching	5	6	1	1-C=O+1-OOH+1-ONO_2	4.1589E-07
702	Branching	6	6	1	1-C=O+1-OOH+1-ONO_2	1.3598E-07

703	Branching	7	6	1	1-C=O+1-OOH+1-ONO_2	4.4464E-08
704	Branching	8	6	1	1-C=O+1-OOH+1-ONO_2	1.4538E-08
705	Branching	9	6	1	1-C=O+1-OOH+1-ONO_2	4.7537E-09
706	Branching	10	6	1	1-C=O+1-OOH+1-ONO_2	1.5543E-09
707	Branching	11	6	1	1-C=O+1-OOH+1-ONO_2	5.0823E-10
708	Branching	12	6	1	1-C=O+1-OOH+1-ONO_2	1.6618E-10
709	Branching	13	6	1	1-C=O+1-OOH+1-ONO_2	5.4336E-11
710	Branching	14	6	1	1-C=O+1-OOH+1-ONO_2	1.7767E-11
711	Branching	5	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	3.1661E-09
712	Branching	6	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.0352E-09
713	Branching	7	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	3.3849E-10
714	Branching	8	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.1068E-10
715	Branching	9	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	3.6189E-11
716	Branching	10	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.1833E-11
717	Branching	11	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	3.8691E-12
718	Branching	12	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.2651E-12
719	Branching	13	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	4.1365E-13
720	Branching	14	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.3525E-13
721	Cyclo	5	0	0	-	4.0976E-01
722	Cyclo	6	0	0	-	1.3398E-01
723	Cyclo	7	0	0	-	4.3809E-02
724	Cyclo	8	0	0	-	1.4324E-02
725	Cyclo	9	0	0	-	4.6837E-03
726	Cyclo	10	0	0	-	1.5315E-03
727	Cyclo	11	0	0	-	5.0075E-04
728	Cyclo	12	0	0	-	1.6373E-04
729	Cyclo	13	0	0	-	5.3536E-05
730	Cyclo	14	0	0	-	1.7505E-05
731	Cyclo	5	1	0	1-OH	8.2274E-03
732	Cyclo	6	1	0	1-OH	2.6902E-03
733	Cyclo	7	1	0	1-OH	8.7961E-04
734	Cyclo	8	1	0	1-OH	2.8761E-04
735	Cyclo	9	1	0	1-OH	9.4042E-05
736	Cyclo	10	1	0	1-OH	3.0749E-05
737	Cyclo	11	1	0	1-OH	1.0054E-05
738	Cyclo	12	1	0	1-OH	3.2875E-06
739	Cyclo	13	1	0	1-OH	1.0749E-06
740	Cyclo	14	1	0	1-OH	3.5147E-07
741	Cyclo	5	2	0	2-OH	1.9014E-05
742	Cyclo	6	2	0	2-OH	6.2171E-06
743	Cyclo	7	2	0	2-OH	2.0328E-06

744	Cyclo	8	2	0	2-OH	6.6468E-07
745	Cyclo	9	2	0	2-OH	2.1733E-07
746	Cyclo	10	2	0	2-OH	7.1063E-08
747	Cyclo	11	2	0	2-OH	2.3236E-08
748	Cyclo	12	2	0	2-OH	7.5975E-09
749	Cyclo	13	2	0	2-OH	2.4842E-09
750	Cyclo	14	2	0	2-OH	8.1227E-10
751	Cyclo	5	3	0	3-OH	3.2544E-08
752	Cyclo	6	3	0	3-OH	1.0641E-08
753	Cyclo	7	3	0	3-OH	3.4794E-09
754	Cyclo	8	3	0	3-OH	1.1377E-09
755	Cyclo	9	3	0	3-OH	3.7199E-10
756	Cyclo	10	3	0	3-OH	1.2163E-10
757	Cyclo	11	3	0	3-OH	3.9771E-11
758	Cyclo	12	3	0	3-OH	1.3004E-11
759	Cyclo	13	3	0	3-OH	4.2520E-12
760	Cyclo	14	3	0	3-OH	1.3903E-12
761	Cyclo	5	1	0	1-C=O	2.6148E-02
762	Cyclo	6	1	0	1-C=O	8.5498E-03
763	Cyclo	7	1	0	1-C=O	2.7956E-03
764	Cyclo	8	1	0	1-C=O	9.1408E-04
765	Cyclo	9	1	0	1-C=O	2.9888E-04
766	Cyclo	10	1	0	1-C=O	9.7726E-05
767	Cyclo	11	1	0	1-C=O	3.1954E-05
768	Cyclo	12	1	0	1-C=O	1.0448E-05
769	Cyclo	13	1	0	1-C=O	3.4163E-06
770	Cyclo	14	1	0	1-C=O	1.1170E-06
771	Cyclo	5	2	0	2-C=O	2.3716E-03
772	Cyclo	6	2	0	2-C=O	7.7546E-04
773	Cyclo	7	2	0	2-C=O	2.5355E-04
774	Cyclo	8	2	0	2-C=O	8.2906E-05
775	Cyclo	9	2	0	2-C=O	2.7108E-05
776	Cyclo	10	2	0	2-C=O	8.8637E-06
777	Cyclo	11	2	0	2-C=O	2.8982E-06
778	Cyclo	12	2	0	2-C=O	9.4764E-07
779	Cyclo	13	2	0	2-C=O	3.0985E-07
780	Cyclo	14	2	0	2-C=O	1.0131E-07
781	Cyclo	5	3	0	3-C=O	3.1162E-04
782	Cyclo	6	3	0	3-C=O	1.0189E-04
783	Cyclo	7	3	0	3-C=O	3.3316E-05
784	Cyclo	8	3	0	3-C=O	1.0894E-05
785	Cyclo	9	3	0	3-C=O	3.5619E-06
786	Cyclo	10	3	0	3-C=O	1.1647E-06
787	Cyclo	11	3	0	3-C=O	3.8081E-07

788	Cyclo	12	3	0	3-C=O	1.2452E-07
789	Cyclo	13	3	0	3-C=O	4.0714E-08
790	Cyclo	14	3	0	3-C=O	1.3312E-08
791	Cyclo	5	2	0	1-OOH	6.0751E-04
792	Cyclo	6	2	0	1-OOH	1.9864E-04
793	Cyclo	7	2	0	1-OOH	6.4951E-05
794	Cyclo	8	2	0	1-OOH	2.1237E-05
795	Cyclo	9	2	0	1-OOH	6.9440E-06
796	Cyclo	10	2	0	1-OOH	2.2705E-06
797	Cyclo	11	2	0	1-OOH	7.4240E-07
798	Cyclo	12	2	0	1-OOH	2.4275E-07
799	Cyclo	13	2	0	1-OOH	7.9372E-08
800	Cyclo	14	2	0	1-OOH	2.5953E-08
801	Cyclo	5	4	0	2-OOH	3.1306E-07
802	Cyclo	6	4	0	2-OOH	1.0236E-07
803	Cyclo	7	4	0	2-OOH	3.3470E-08
804	Cyclo	8	4	0	2-OOH	1.0944E-08
805	Cyclo	9	4	0	2-OOH	3.5784E-09
806	Cyclo	10	4	0	2-OOH	1.1700E-09
807	Cyclo	11	4	0	2-OOH	3.8257E-10
808	Cyclo	12	4	0	2-OOH	1.2509E-10
809	Cyclo	13	4	0	2-OOH	4.0902E-11
810	Cyclo	14	4	0	2-OOH	1.3374E-11
811	Cyclo	5	6	0	3-OOH	1.3558E-10
812	Cyclo	6	6	0	3-OOH	4.4331E-11
813	Cyclo	7	6	0	3-OOH	1.4495E-11
814	Cyclo	8	6	0	3-OOH	4.7395E-12
815	Cyclo	9	6	0	3-OOH	1.5497E-12
816	Cyclo	10	6	0	3-OOH	5.0671E-13
817	Cyclo	11	6	0	3-OOH	1.6568E-13
818	Cyclo	12	6	0	3-OOH	5.4174E-14
819	Cyclo	13	6	0	3-OOH	1.7713E-14
820	Cyclo	14	6	0	3-OOH	5.7919E-15
821	Cyclo	5	3	1	1-ONO_2	1.7551E-03
822	Cyclo	6	3	1	1-ONO_2	5.7387E-04
823	Cyclo	7	3	1	1-ONO_2	1.8764E-04
824	Cyclo	8	3	1	1-ONO_2	6.1354E-05
825	Cyclo	9	3	1	1-ONO_2	2.0061E-05
826	Cyclo	10	3	1	1-ONO_2	6.5595E-06
827	Cyclo	11	3	1	1-ONO_2	2.1448E-06
828	Cyclo	12	3	1	1-ONO_2	7.0130E-07
829	Cyclo	13	3	1	1-ONO_2	2.2931E-07

830	Cyclo	14	3	1	1-ONO_2	7.4978E-08
831	Cyclo	5	6	2	2-ONO_2	7.5175E-06
832	Cyclo	6	6	2	2-ONO_2	2.4580E-06
833	Cyclo	7	6	2	2-ONO_2	8.0371E-07
834	Cyclo	8	6	2	2-ONO_2	2.6279E-07
835	Cyclo	9	6	2	2-ONO_2	8.5927E-08
836	Cyclo	10	6	2	2-ONO_2	2.8096E-08
837	Cyclo	11	6	2	2-ONO_2	9.1867E-09
838	Cyclo	12	6	2	2-ONO_2	3.0038E-09
839	Cyclo	13	6	2	2-ONO_2	9.8217E-10
840	Cyclo	14	6	2	2-ONO_2	3.2115E-10
841	Cyclo	5	9	3	3-ONO_2	3.2199E-08
842	Cyclo	6	9	3	3-ONO_2	1.0528E-08
843	Cyclo	7	9	3	3-ONO_2	3.4425E-09
844	Cyclo	8	9	3	3-ONO_2	1.1256E-09
845	Cyclo	9	9	3	3-ONO_2	3.6805E-10
846	Cyclo	10	9	3	3-ONO_2	1.2034E-10
847	Cyclo	11	9	3	3-ONO_2	3.9349E-11
848	Cyclo	12	9	3	3-ONO_2	1.2866E-11
849	Cyclo	13	9	3	3-ONO_2	4.2069E-12
850	Cyclo	14	9	3	3-ONO_2	1.3755E-12
851	Cyclo	5	2	0	1-OH+1-C=O	5.2502E-04
852	Cyclo	6	2	0	1-OH+1-C=O	1.7167E-04
853	Cyclo	7	2	0	1-OH+1-C=O	5.6131E-05
854	Cyclo	8	2	0	1-OH+1-C=O	1.8353E-05
855	Cyclo	9	2	0	1-OH+1-C=O	6.0011E-06
856	Cyclo	10	2	0	1-OH+1-C=O	1.9622E-06
857	Cyclo	11	2	0	1-OH+1-C=O	6.4159E-07
858	Cyclo	12	2	0	1-OH+1-C=O	2.0978E-07
859	Cyclo	13	2	0	1-OH+1-C=O	6.8594E-08
860	Cyclo	14	2	0	1-OH+1-C=O	2.2429E-08
861	Cyclo	5	3	0	1-OH+1-OOH	4.6249E-06
862	Cyclo	6	3	0	1-OH+1-OOH	1.5122E-06
863	Cyclo	7	3	0	1-OH+1-OOH	4.9446E-07
864	Cyclo	8	3	0	1-OH+1-OOH	1.6168E-07
865	Cyclo	9	3	0	1-OH+1-OOH	5.2864E-08
866	Cyclo	10	3	0	1-OH+1-OOH	1.7285E-08
867	Cyclo	11	3	0	1-OH+1-OOH	5.6518E-09
868	Cyclo	12	3	0	1-OH+1-OOH	1.8480E-09
869	Cyclo	13	3	0	1-OH+1-OOH	6.0425E-10
870	Cyclo	14	3	0	1-OH+1-OOH	1.9757E-10

871	Cyclo	5	4	1	1-OH+1-ONO_2	3.5240E-05
872	Cyclo	6	4	1	1-OH+1-ONO_2	1.1523E-05
873	Cyclo	7	4	1	1-OH+1-ONO_2	3.7676E-06
874	Cyclo	8	4	1	1-OH+1-ONO_2	1.2319E-06
875	Cyclo	9	4	1	1-OH+1-ONO_2	4.0280E-07
876	Cyclo	10	4	1	1-OH+1-ONO_2	1.3171E-07
877	Cyclo	11	4	1	1-OH+1-ONO_2	4.3065E-08
878	Cyclo	12	4	1	1-OH+1-ONO_2	1.4081E-08
879	Cyclo	13	4	1	1-OH+1-ONO_2	4.6041E-09
880	Cyclo	14	4	1	1-OH+1-ONO_2	1.5054E-09
881	Cyclo	5	3	0	1-C=O+1-OOH	3.8767E-05
882	Cyclo	6	3	0	1-C=O+1-OOH	1.2676E-05
883	Cyclo	7	3	0	1-C=O+1-OOH	4.1447E-06
884	Cyclo	8	3	0	1-C=O+1-OOH	1.3552E-06
885	Cyclo	9	3	0	1-C=O+1-OOH	4.4312E-07
886	Cyclo	10	3	0	1-C=O+1-OOH	1.4489E-07
887	Cyclo	11	3	0	1-C=O+1-OOH	4.7375E-08
888	Cyclo	12	3	0	1-C=O+1-OOH	1.5490E-08
889	Cyclo	13	3	0	1-C=O+1-OOH	5.0650E-09
890	Cyclo	14	3	0	1-C=O+1-OOH	1.6561E-09
891	Cyclo	5	4	1	1-C=O+1-ONO_2	1.1200E-04
892	Cyclo	6	4	1	1-C=O+1-ONO_2	3.6621E-05
893	Cyclo	7	4	1	1-C=O+1-ONO_2	1.1974E-05
894	Cyclo	8	4	1	1-C=O+1-ONO_2	3.9152E-06
895	Cyclo	9	4	1	1-C=O+1-ONO_2	1.2802E-06
896	Cyclo	10	4	1	1-C=O+1-ONO_2	4.1858E-07
897	Cyclo	11	4	1	1-C=O+1-ONO_2	1.3687E-07
898	Cyclo	12	4	1	1-C=O+1-ONO_2	4.4752E-08
899	Cyclo	13	4	1	1-C=O+1-ONO_2	1.4633E-08
900	Cyclo	14	4	1	1-C=O+1-ONO_2	4.7845E-09
901	Cyclo	5	5	1	1-OOH+1-ONO_2	2.6021E-06
902	Cyclo	6	5	1	1-OOH+1-ONO_2	8.5083E-07
903	Cyclo	7	5	1	1-OOH+1-ONO_2	2.7820E-07
904	Cyclo	8	5	1	1-OOH+1-ONO_2	9.0964E-08
905	Cyclo	9	5	1	1-OOH+1-ONO_2	2.9743E-08
906	Cyclo	10	5	1	1-OOH+1-ONO_2	9.7252E-09
907	Cyclo	11	5	1	1-OOH+1-ONO_2	3.1799E-09
908	Cyclo	12	5	1	1-OOH+1-ONO_2	1.0397E-09
909	Cyclo	13	5	1	1-OOH+1-ONO_2	3.3997E-10
910	Cyclo	14	5	1	1-OOH+1-ONO_2	1.1116E-10

911	Cyclo	5	3	0	2-OH+1-C=O	1.05E-06
912	Cyclo	6	3	0	2-OH+1-C=O	3.43E-07
913	Cyclo	7	3	0	2-OH+1-C=O	1.12E-07
914	Cyclo	8	3	0	2-OH+1-C=O	3.67E-08
915	Cyclo	9	3	0	2-OH+1-C=O	1.20E-08
916	Cyclo	10	3	0	2-OH+1-C=O	3.92E-09
917	Cyclo	11	3	0	2-OH+1-C=O	1.28E-09
918	Cyclo	12	3	0	2-OH+1-C=O	4.19E-10
919	Cyclo	13	3	0	2-OH+1-C=O	1.37E-10
920	Cyclo	14	3	0	2-OH+1-C=O	4.48E-11
921	Cyclo	5	4	0	2-OH+1-OOH	7.07E-09
922	Cyclo	6	4	0	2-OH+1-OOH	2.31E-09
923	Cyclo	7	4	0	2-OH+1-OOH	7.56E-10
924	Cyclo	8	4	0	2-OH+1-OOH	2.47E-10
925	Cyclo	9	4	0	2-OH+1-OOH	8.09E-11
926	Cyclo	10	4	0	2-OH+1-OOH	2.64E-11
927	Cyclo	11	4	0	2-OH+1-OOH	8.64E-12
928	Cyclo	12	4	0	2-OH+1-OOH	2.83E-12
929	Cyclo	13	4	0	2-OH+1-OOH	9.24E-13
930	Cyclo	14	4	0	2-OH+1-OOH	3.02E-13
931	Cyclo	5	5	1	2-OH+1-ONO_2	7.04E-08
932	Cyclo	6	5	1	2-OH+1-ONO_2	2.30E-08
933	Cyclo	7	5	1	2-OH+1-ONO_2	7.53E-09
934	Cyclo	8	5	1	2-OH+1-ONO_2	2.46E-09
935	Cyclo	9	5	1	2-OH+1-ONO_2	8.05E-10
936	Cyclo	10	5	1	2-OH+1-ONO_2	2.63E-10
937	Cyclo	11	5	1	2-OH+1-ONO_2	8.61E-11
938	Cyclo	12	5	1	2-OH+1-ONO_2	2.81E-11
939	Cyclo	13	5	1	2-OH+1-ONO_2	9.20E-12
940	Cyclo	14	5	1	2-OH+1-ONO_2	3.01E-12
941	Cyclo	5	3	0	2-C=O+1-OH	8.65E-05
942	Cyclo	6	3	0	2-C=O+1-OH	2.83E-05
943	Cyclo	7	3	0	2-C=O+1-OH	9.24E-06
944	Cyclo	8	3	0	2-C=O+1-OH	3.02E-06
945	Cyclo	9	3	0	2-C=O+1-OH	9.88E-07
946	Cyclo	10	3	0	2-C=O+1-OH	3.23E-07
947	Cyclo	11	3	0	2-C=O+1-OH	1.06E-07
948	Cyclo	12	3	0	2-C=O+1-OH	3.45E-08
949	Cyclo	13	3	0	2-C=O+1-OH	1.13E-08
950	Cyclo	14	3	0	2-C=O+1-OH	3.69E-09
951	Cyclo	5	4	0	2-C=O+1-OOH	6.38E-06
952	Cyclo	6	4	0	2-C=O+1-OOH	2.09E-06

953	Cyclo	7	4	0	2-C=O+1-OOH	6.83E-07
954	Cyclo	8	4	0	2-C=O+1-OOH	2.23E-07
955	Cyclo	9	4	0	2-C=O+1-OOH	7.30E-08
956	Cyclo	10	4	0	2-C=O+1-OOH	2.39E-08
957	Cyclo	11	4	0	2-C=O+1-OOH	7.80E-09
958	Cyclo	12	4	0	2-C=O+1-OOH	2.55E-09
959	Cyclo	13	4	0	2-C=O+1-OOH	8.34E-10
960	Cyclo	14	4	0	2-C=O+1-OOH	2.73E-10
961	Cyclo	5	5	1	2-C=O+1-ONO_2	1.84E-05
962	Cyclo	6	5	1	2-C=O+1-ONO_2	6.03E-06
963	Cyclo	7	5	1	2-C=O+1-ONO_2	1.97E-06
964	Cyclo	8	5	1	2-C=O+1-ONO_2	6.45E-07
965	Cyclo	9	5	1	2-C=O+1-ONO_2	2.11E-07
966	Cyclo	10	5	1	2-C=O+1-ONO_2	6.89E-08
967	Cyclo	11	5	1	2-C=O+1-ONO_2	2.25E-08
968	Cyclo	12	5	1	2-C=O+1-ONO_2	7.37E-09
969	Cyclo	13	5	1	2-C=O+1-ONO_2	2.41E-09
970	Cyclo	14	5	1	2-C=O+1-ONO_2	7.88E-10
971	Cyclo	5	5	0	2-OOH+1-OH	2.08E-09
972	Cyclo	6	5	0	2-OOH+1-OH	6.81E-10
973	Cyclo	7	5	0	2-OOH+1-OH	2.23E-10
974	Cyclo	8	5	0	2-OOH+1-OH	7.28E-11
975	Cyclo	9	5	0	2-OOH+1-OH	2.38E-11
976	Cyclo	10	5	0	2-OOH+1-OH	7.78E-12
977	Cyclo	11	5	0	2-OOH+1-OH	2.54E-12
978	Cyclo	12	5	0	2-OOH+1-OH	8.32E-13
979	Cyclo	13	5	0	2-OOH+1-OH	2.72E-13
980	Cyclo	14	5	0	2-OOH+1-OH	8.89E-14
981	Cyclo	5	5	0	2-OOH+1-C=O	2.00E-08
982	Cyclo	6	5	0	2-OOH+1-C=O	6.53E-09
983	Cyclo	7	5	0	2-OOH+1-C=O	2.14E-09
984	Cyclo	8	5	0	2-OOH+1-C=O	6.98E-10
985	Cyclo	9	5	0	2-OOH+1-C=O	2.28E-10
986	Cyclo	10	5	0	2-OOH+1-C=O	7.47E-11
987	Cyclo	11	5	0	2-OOH+1-C=O	2.44E-11
988	Cyclo	12	5	0	2-OOH+1-C=O	7.98E-12
989	Cyclo	13	5	0	2-OOH+1-C=O	2.61E-12
990	Cyclo	14	5	0	2-OOH+1-C=O	8.53E-13
991	Cyclo	5	7	1	2-OOH+1-ONO_2	1.34E-09
992	Cyclo	6	7	1	2-OOH+1-ONO_2	4.38E-10
993	Cyclo	7	7	1	2-OOH+1-ONO_2	1.43E-10
994	Cyclo	8	7	1	2-OOH+1-ONO_2	4.69E-11

995	Cyclo	9	7	1	2-OOH+1-ONO_2	1.53E-11
996	Cyclo	10	7	1	2-OOH+1-ONO_2	5.01E-12
997	Cyclo	11	7	1	2-OOH+1-ONO_2	1.64E-12
998	Cyclo	12	7	1	2-OOH+1-ONO_2	5.36E-13
999	Cyclo	13	7	1	2-OOH+1-ONO_2	1.75E-13
1000	Cyclo	14	7	1	2-OOH+1-ONO_2	5.73E-14
1001	Cyclo	5	7	2	2-ONO_2+1-OH	1.51E-07
1002	Cyclo	6	7	2	2-ONO_2+1-OH	4.94E-08
1003	Cyclo	7	7	2	2-ONO_2+1-OH	1.61E-08
1004	Cyclo	8	7	2	2-ONO_2+1-OH	5.28E-09
1005	Cyclo	9	7	2	2-ONO_2+1-OH	1.73E-09
1006	Cyclo	10	7	2	2-ONO_2+1-OH	5.64E-10
1007	Cyclo	11	7	2	2-ONO_2+1-OH	1.84E-10
1008	Cyclo	12	7	2	2-ONO_2+1-OH	6.03E-11
1009	Cyclo	13	7	2	2-ONO_2+1-OH	1.97E-11
1010	Cyclo	14	7	2	2-ONO_2+1-OH	6.45E-12
1011	Cyclo	5	7	2	2-ONO_2+1-C=O	4.80E-07
1012	Cyclo	6	7	2	2-ONO_2+1-C=O	1.57E-07
1013	Cyclo	7	7	2	2-ONO_2+1-C=O	5.13E-08
1014	Cyclo	8	7	2	2-ONO_2+1-C=O	1.68E-08
1015	Cyclo	9	7	2	2-ONO_2+1-C=O	5.48E-09
1016	Cyclo	10	7	2	2-ONO_2+1-C=O	1.79E-09
1017	Cyclo	11	7	2	2-ONO_2+1-C=O	5.86E-10
1018	Cyclo	12	7	2	2-ONO_2+1-C=O	1.92E-10
1019	Cyclo	13	7	2	2-ONO_2+1-C=O	6.2675E-11
1020	Cyclo	14	7	2	2-ONO_2+1-C=O	2.0493E-11
1021	Cyclo	5	8	2	2-ONO_2+1-OOH	1.1145E-08
1022	Cyclo	6	8	2	2-ONO_2+1-OOH	3.6443E-09
1023	Cyclo	7	8	2	2-ONO_2+1-OOH	1.1916E-09
1024	Cyclo	8	8	2	2-ONO_2+1-OOH	3.8962E-10
1025	Cyclo	9	8	2	2-ONO_2+1-OOH	1.2740E-10
1026	Cyclo	10	8	2	2-ONO_2+1-OOH	4.1655E-11
1027	Cyclo	11	8	2	2-ONO_2+1-OOH	1.3620E-11
1028	Cyclo	12	8	2	2-ONO_2+1-OOH	4.4535E-12
1029	Cyclo	13	8	2	2-ONO_2+1-OOH	1.4562E-12
1030	Cyclo	14	8	2	2-ONO_2+1-OOH	4.7613E-13
1031	Cyclo	5	4	0	1-OH+1-C=O+1-OOH	2.9513E-07
1032	Cyclo	6	4	0	1-OH+1-C=O+1-OOH	9.6500E-08
1033	Cyclo	7	4	0	1-OH+1-C=O+1-OOH	3.1553E-08

1034	Cyclo	8	4	0	1-OH+1-C=O+1-OOH	1.0317E-08
1035	Cyclo	9	4	0	1-OH+1-C=O+1-OOH	3.3734E-09
1036	Cyclo	10	4	0	1-OH+1-C=O+1-OOH	1.1030E-09
1037	Cyclo	11	4	0	1-OH+1-C=O+1-OOH	3.6066E-10
1038	Cyclo	12	4	0	1-OH+1-C=O+1-OOH	1.1793E-10
1039	Cyclo	13	4	0	1-OH+1-C=O+1-OOH	3.8559E-11
1040	Cyclo	14	4	0	1-OH+1-C=O+1-OOH	1.2608E-11
1041	Cyclo	5	5	1	1-OH+1-C=O+1-ONO_2	2.2488E-06
1042	Cyclo	6	5	1	1-OH+1-C=O+1-ONO_2	7.3529E-07
1043	Cyclo	7	5	1	1-OH+1-C=O+1-ONO_2	2.4042E-07
1044	Cyclo	8	5	1	1-OH+1-C=O+1-ONO_2	7.8611E-08
1045	Cyclo	9	5	1	1-OH+1-C=O+1-ONO_2	2.5704E-08
1046	Cyclo	10	5	1	1-OH+1-C=O+1-ONO_2	8.4046E-09
1047	Cyclo	11	5	1	1-OH+1-C=O+1-ONO_2	2.7481E-09
1048	Cyclo	12	5	1	1-OH+1-C=O+1-ONO_2	8.9855E-10
1049	Cyclo	13	5	1	1-OH+1-C=O+1-ONO_2	2.9380E-10
1050	Cyclo	14	5	1	1-OH+1-C=O+1-ONO_2	9.6066E-11
1051	Cyclo	5	6	1	1-OH+1-OOH+1-ONO_2	1.9809E-08
1052	Cyclo	6	6	1	1-OH+1-OOH+1-ONO_2	6.4772E-09
1053	Cyclo	7	6	1	1-OH+1-OOH+1-ONO_2	2.1179E-09
1054	Cyclo	8	6	1	1-OH+1-OOH+1-ONO_2	6.9249E-10
1055	Cyclo	9	6	1	1-OH+1-OOH+1-ONO_2	2.2643E-10
1056	Cyclo	10	6	1	1-OH+1-OOH+1-ONO_2	7.4036E-11
1057	Cyclo	11	6	1	1-OH+1-OOH+1-ONO_2	2.4208E-11
1058	Cyclo	12	6	1	1-OH+1-OOH+1-ONO_2	7.9154E-12
1059	Cyclo	13	6	1	1-OH+1-OOH+1-ONO_2	2.5881E-12
1060	Cyclo	14	6	1	1-OH+1-OOH+1-ONO_2	8.4625E-13
1061	Cyclo	5	6	1	1-C=O+1-OOH+1-ONO_2	1.6605E-07
1062	Cyclo	6	6	1	1-C=O+1-OOH+1-ONO_2	5.4294E-08
1063	Cyclo	7	6	1	1-C=O+1-OOH+1-ONO_2	1.7753E-08
1064	Cyclo	8	6	1	1-C=O+1-OOH+1-ONO_2	5.8047E-09
1065	Cyclo	9	6	1	1-C=O+1-OOH+1-ONO_2	1.8980E-09
1066	Cyclo	10	6	1	1-C=O+1-OOH+1-ONO_2	6.2059E-10
1067	Cyclo	11	6	1	1-C=O+1-OOH+1-ONO_2	2.0292E-10
1068	Cyclo	12	6	1	1-C=O+1-OOH+1-ONO_2	6.6349E-11
1069	Cyclo	13	6	1	1-C=O+1-OOH+1-ONO_2	2.1694E-11
1070	Cyclo	14	6	1	1-C=O+1-OOH+1-ONO_2	7.0935E-12
1071	Cyclo	5	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.2641E-09
1072	Cyclo	6	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	4.1333E-10

1073	Cyclo	7	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.3515E-10
1074	Cyclo	8	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	4.4190E-11
1075	Cyclo	9	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.4449E-11
1076	Cyclo	10	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	4.7245E-12
1077	Cyclo	11	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.5448E-12
1078	Cyclo	12	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	5.0510E-13
1079	Cyclo	13	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	1.6516E-13
1080	Cyclo	14	7	1	1-OH+1-C=O+1-OOH+1-ONO_2	5.4002E-14

Table S2. Values of best-fit parameters in Equation (2).

Best-fit parameters	Values
n_C^0	2.6212e+01
b_C	4.3909e-01
b_O	1.4606e+00
b_{CO}	1.8457e-02
$b_{(-OH)}$	6.1623e-01
$b_{(-C=O)}$	-6.0560e-01
$b_{(-OOH)}$	-4.7798e-03
$b_{(-ONO2)}$	-2.3032e+00

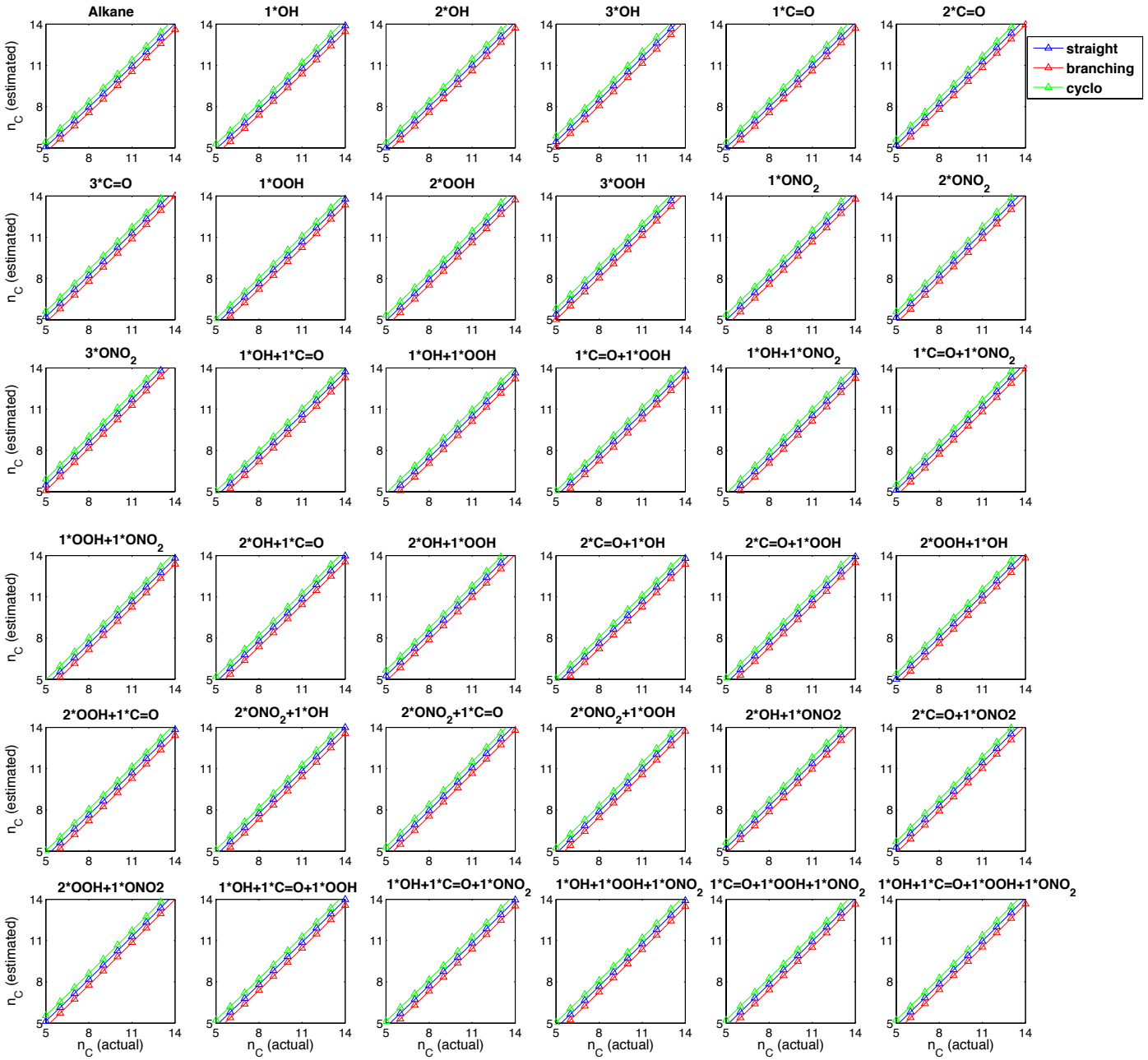

Figure S1. Estimated vs. Actual carbon numbers for 1080 standards.

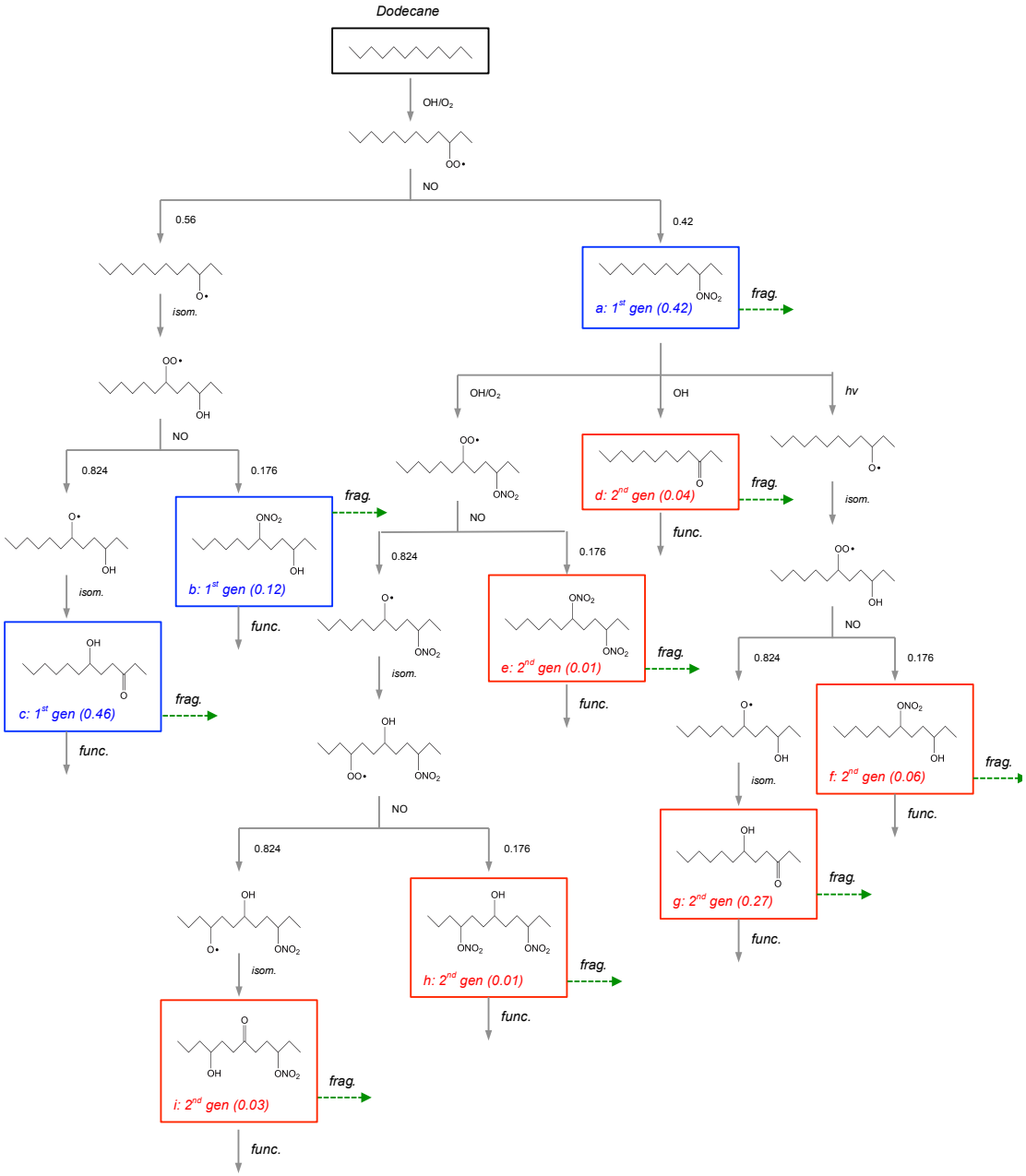

Figure S2. Development of the functionalization vs. fragmentation channels in the FGOM model, using the high-NO_x photooxidation of dodecane as an example.

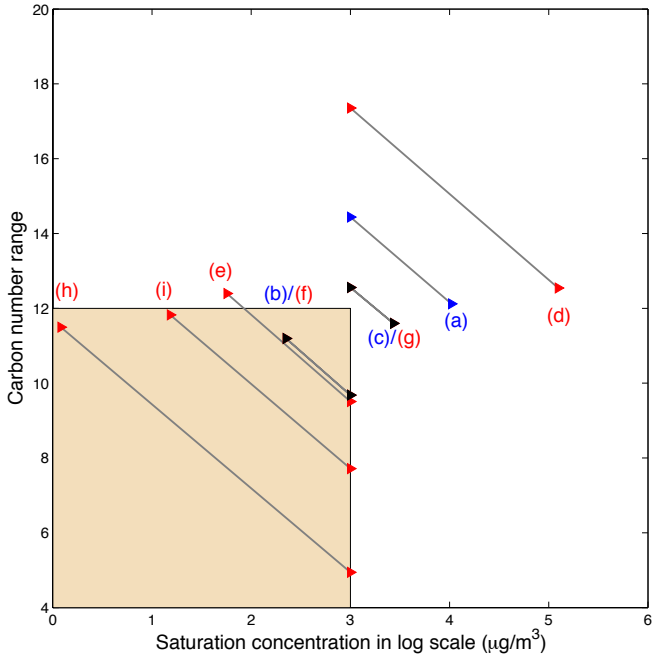

Figure S3. Carbon number range for 1st and 2nd generation products of OH oxidation of dodecane under high-NO_x conditions. For illustration, the shaded region ($C^* \leq 1000$ $\mu g/m^3$) is taken to represent the combination of carbon number and volatility for which a molecule can appreciably partition to the particle phase.